

Normal heat conduction in lattice models with asymmetry harmonic interparticle interactions.

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We study the heat conduct behavior of a lattice model with asymmetry harmonic inter-particle interactions in this paper. Normal heat conductivity independent of the system size is observed when the lattice chain is long enough. Because only the harmonic interactions are involved, the result confirms without ambiguous interpretation that the asymmetry plays the key role in resulting in the normal heat conduct of one dimensional momentum conserving lattices. Both equilibrium and non-equilibrium simulations are performed to support the conclusion.

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The heat transport properties of low-dimensional systems have evoked intensive studies for decades [1-13], aiming at to verify whether the Fourier's law of heat conduction

$$J = -\kappa \nabla T \quad (1)$$

valid in low-dimensional materials. Here J is the heat current, ∇T is the temperature gradient along the sample, κ is the thermal conductivity. At present, for momentum-conserving 1D fluids and lattices, it is generally believed that the thermal conductivity should diverge as $\kappa \sim L^\alpha$ with the increase of the system size L for momentum conserving low-dimensional systems[14-19]. Meanwhile, some counterexamples with size-independent thermal conductivities have been also found, such as the rotator model [20,21], a 1D lattice in effective magnetic fields [22], the variant ding-a-ling model [23].

Recently we find that momentum-conserved lattice models with asymmetric interparticle interactions [24] can also result the normal heat conduction. This result is confirmed by investigating the time-dependent behavior of current autocorrelation functions in one-dimensional lattice systems with the asymmetric and symmetric interaction potentials [25]. The current autocorrelation is defined as

$$C(t) = \langle J(t)J(0) \rangle,$$

where $J(t)$ represents the current fluctuation at time t and Here $\langle \cdot \rangle$ denotes the equilibrium thermodynamic average. Following the linear response theory [27], the thermal conductivity may be calculated by the Green-Kubo formula

$$\kappa = \lim_{\tau \rightarrow \infty} \lim_{N \rightarrow \infty} \frac{1}{2k_B T} \int_0^\tau C(t) dt, \quad (2)$$

once the correlation function $C(t)$ is obtained, where τ is the time of evolution, L is the linear dimension of the system along which the current flows, k_B is the Boltzmann constant, T is the temperature of the system. Differing from the direct nonequilibrium calculation based on

equation (1), the thermal conductivity here is calculated with current fluctuations in the equilibrium system. After studying different types of interaction potentials, it is found [25] that with proper degree of asymmetry, the current autocorrelation may show rapid decay which led to the convergence of the Green-Kubo formula.

It is well-known that the asymmetry interaction may induce the thermal expansion while the symmetry one may not, and real materials usually show thermal expansion effect[26]. Thus, our finding has particular importance for real materials. It implies that low-dimensional materials may also have the size-independent thermal conductivity in the thermal limit as the bulk materials, and the Fourier's law of heat conduction is generally valid also for low-dimensional materials. However, as mentioned above, at present it is generally accepted that the heat current autocorrelation decays in power-law and the thermal conductivity diverges with the system size in one-dimensional momentum conserving systems. Meanwhile, the models we have studied [25,26] have a combination potential of nonlinearity and asymmetry. Therefore, whether the convergent thermal conductivity is resulted by the nonlinearity or the asymmetry feature needs to be clarified. This paper studies an one-dimensional momentum conserving lattice with simple asymmetric interparticle interactions: The compress and stretch are govern by different harmonic potentials. In more detail, we study the lattice described by the Hamiltonian

$$H = \sum_{i=1}^N \frac{p_i^2}{2} + V(x_i - x_{i-1}), \quad (3)$$

where p_i and x_i represent the momentum and the deviation from its equilibrium position of the i th particle respectively. The potential is as following:

$$V(x) = \begin{cases} \frac{1}{2}(1+r)x^2 & \text{if } x < 0, \\ \frac{1}{2}(1-r)x^2 & \text{otherwise.} \end{cases} \quad (4)$$

where r control the degree of the asymmetry. The potentials with several r are plotted in Fig.1. This potential

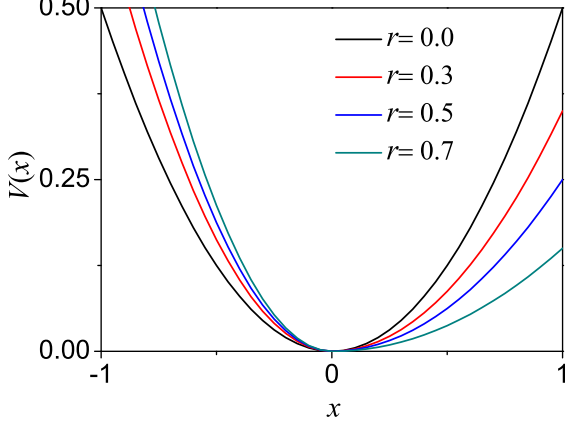


FIG. 1: plot of asymmetric harmonic interaction potential with $r = 0.0$, $r = 0.3$, $r = 0.5$ and $r = 0.7$.

and its higher order derivatives are continuous at $x = 0$ except the second derivative.

To perform the nonequilibrium simulations, the Nose-Hoover heat baths [28] with temperatures T_L and T_R are coupled to the left and right particles respectively. The fixed boundary conditions are applied in the simulation. The equations of the motion of particles in heat baths is given by

$$\dot{x}_{1,N} = \frac{p_{1,N}}{\mu}, \quad \dot{p}_{1,N} = -\frac{\partial H}{\partial x_{1,N}} - \zeta_{\pm} p_{1,N}, \quad \dot{\zeta}_{\pm} = \frac{p_{\pm}^2}{T_{\pm}} - 1, \quad (5)$$

and the motions of $N - 2$ other particles are described by

$$\dot{x}_i = \frac{p_i}{\mu}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}. \quad (6)$$

We integrate the equations of motion by using the leapfrog integrating algorithm. The local temperature and local heat current at the i th site are calculated by $T_i \equiv \langle p_i^2 \rangle$ and $J_i \equiv \langle \dot{x}_i \frac{\partial H}{\partial x_i} \rangle$ respectively [8]. The simulations are performed with a sufficient long time, usually $t > 10^7$, to ensure the system reaching a stationary state. In such a state, the local current is equal to the global flux, $J_i = J$. To avoid the finite-size effect, the system size N is extended until the temperature profiles would fit with each other by rescaling the x variable with factor $1/N$, in which case $dT/dx \sim N/(T_L - T_R)$ and the thermal conductivity can thus be calculated following $\kappa = \langle J \rangle N / (T_L - T_R)$.

Figure 2(a) shows the temperature profiles with $r = 0.5$ for several system sizes. One can see that for $N > 10^4$ the temperature profiles are well-rescaled together. Figure 2 (b) shows the thermal conductivity as a function of the system size. It can be seen that κ converges to

be a size-independent constant gradually. A remarkable difference to the case of models with symmetry potential, such as the results shown in refs. [4-7,10,24] where the finite-size effect disappears usually before $N > 10^3$, is that the convergence threshold of the system size is quite long in this model. This feature appears also in our previous work [24,25] where a different asymmetry interaction potential is applied. We guess it may be one of the reason why previous researchers have not observed convergent thermal conductivity even they also investigated certain asymmetry-potential lattice models.

The convergence threshold is related to the degree of the asymmetry. In Fig. 2, we also show the results with $r = 0.3$ and $r = 0.7$ respectively. It is clear that the threshold of convergent thermal conductivity increases with the decrease of the asymmetry degree. However, further increase r may result simulation difficult. We have to apply a very small intergral step to guarantee the integral precision.

As in reference [24], we calculate the mass density $\rho(x)$ along the lattice chain at non-equilibrium stationary states. The results are shown in Fig. 2(c). It can be seen that mass gradients do set up along the chain in the asymmetry cases, while in the symmetry case of $r = 0$ there is no such a gradient. The density is inverse proportional to the temperature. This is a result of positive r , in which case the compress is difficult than the stretch. If one apply a negative r to the potential, in which case the compress is easy than the stretch, he shall found that the mass desity is proportional to the temperature. This is a qualitative different property between symmetry and asymmetry lattice systems, and may provide clue to understand why qualitative difference in heat transport is resulted. We guess that the mass gradient can induce additional scattering of the current and, together with other scattering mechanism, result the normal heat conduct behavior.

The decay behavior of the current autocorrelation can further confirm that the asymmetry interparticle interactions may result the normal heat conduct of lattice systems. To calculate the current autocorrelation function, we first evolve the system for a sufficient long time to relax the system to its equilibrium state. Then the correlation function $C(t) = \langle J(t)J(0) \rangle$ is calculated by applying the emporal current fluctuations $J(t) = \sum_{i=1}^N J_i(t)$. The decay behavior of $C(t)$ determines whether the heat flux violates the Fourier law of heat conduction. If it decays as $C(t) \sim t^{-\gamma}$ with $\gamma < 1$, the κ will divergent following the Green-Kubo formula. If it decays faster than $\gamma = 1$, particularly with exponential decay of $C(t) \sim e^{-\delta t}$, the Green-Kubo formula converges and the thermal conductivity is size-indepdent in the thermodynamical limit. The Fourier law is thus obeyed. Figure 3 shows the current autocorrelation functions corresponding to the parameter sets applied in Fig. 2. To perform the sim-

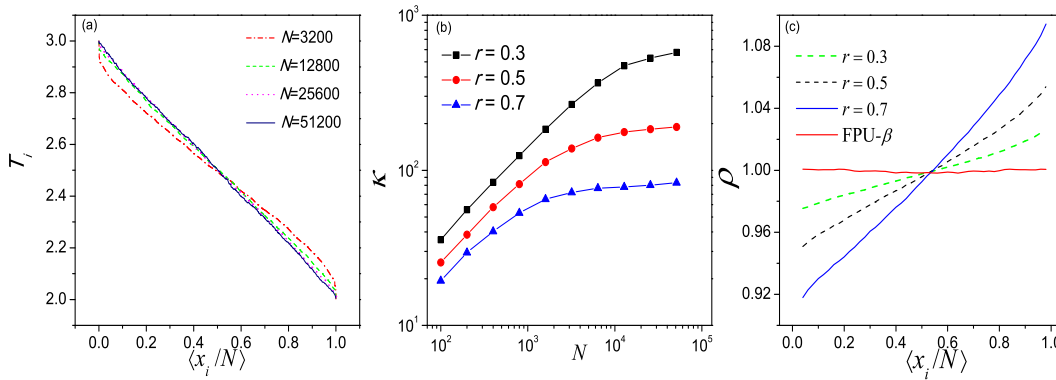


FIG. 2: (a) Temperature profiles for the asymmetric harmonic interaction potential with fixed $r = 0.5$. The temperatures of the two heat baths coupled to the system are $T_L = 3$ and $T_R = 2$ respectively, (b) The heat conductivity κ vs the number of particles N for $r = 0.3$, $r = 0.5$ and $r = 0.7$, (c) The mass density function respectively for the asymmetric harmonic interaction potential model with fixed $r = 0.3$, $r = 0.5$ and $r = 0.7$ and the Fermi-Pasta-Ulam- β (FPU- β) model. The system size is $N = 2000$. Other parameters are $T_L = 3$ and $T_R = 2$.

ulation, periodic boundary conditions are applied with several simulation sizes. The temperature is set to be $T = 2.5$ which is corresponding to the average temperature applied in the nonequilibrium simulations. One may see that the curves with different simulation sizes overlap with each other, indicating that the finite-size effect is avoided. It is clear, either with the log-log plot or semi-log plot, the decay of the autocorrelation function is quite fast, even approaches the exponential decay manner, indicating a convergent thermal conductivity.

In conclusion, the lattice model even with asymmetric harmonic inter-particle interactions shows normal thermal conduction behavior. Our nonequilibrium simulations obtain a size-independent thermal conductivity when the simulation size is sufficient long. Our equilibrium simulations show that the current autocorrelation decay faster than the power-law decay of $C(t) \sim t^{-1}$, implying a convergent thermal conductivity according to the Green-Kubo formula. Because this model involves only the asymmetric harmonic interactions, our results thus confirm that it is the asymmetry of interaction potentials resulting the normal thermal conduct behavior of one-dimensional momentum conserving lattices.

This model has another obvious advantage. With a scale transformation $(\tilde{x}, \tilde{t}) \rightarrow (\alpha x, t)$, the Hamiltonian changes as $\tilde{H} \rightarrow \alpha^2 H$. Therefore, the dynamics of the system keep unchange with the scale transformation. In more detail, the systems with Hamiltonian \tilde{H} at temperature \tilde{T} and with Hamiltonian H at temperature T are identical, where $\tilde{T} = \alpha^2 T$. Therefore, the conclusion of normal thermal conductivity can be directly extended to any temperature.

We have observed that the mass density is set up alone the lattice chain in the case of asymmetry potentials.

This phenomenon may be important in understanding the microscopic mechanism of the normal thermal conductivity in nonequilibrium systems. In equilibrium systems, there is no such a stationary gradient of mass density. How a rapid decay of the current autocorrelation is arisen is an open problem and asks further studies.

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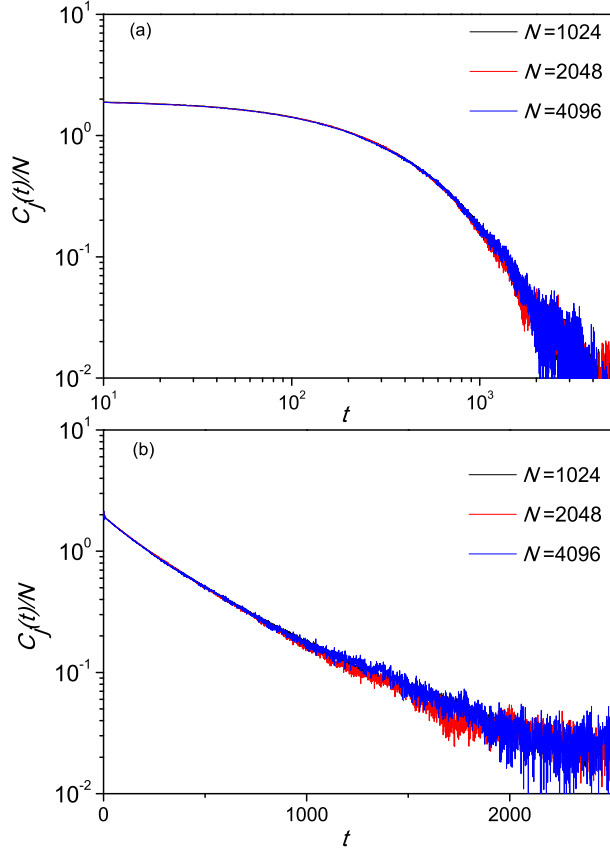


FIG. 3: The autocorrelation function of the heat flux, $C_j(t)$, for the asymmetric harmonic interaction potential with $r = 0.5$.

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